On the Scalability of the *Albany/FELIX* First-Order Stokes Approximation Ice Sheet Solver for Large-Scale Simulations of the Greenland and Antarctic Ice Sheets

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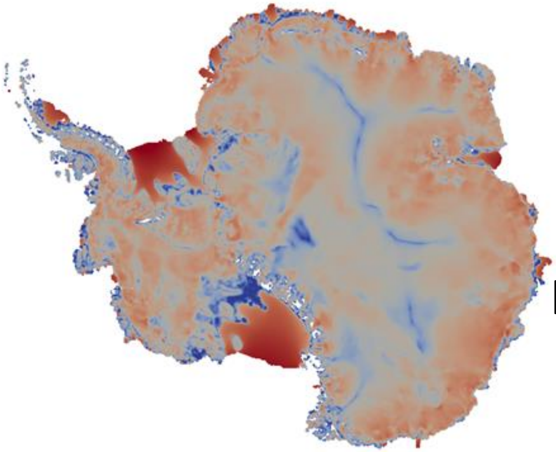

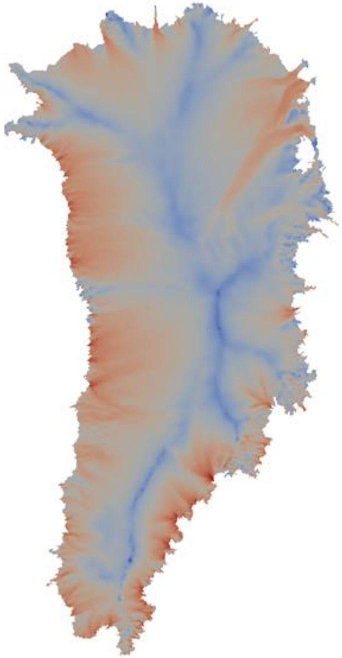

Numerical and Computational Developments to Advance Multiscale Earth System Models (MSESM)

International Conference on Computational Science (ICCS) 2015
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Reykjavik, Iceland

SAND2015-3862C

Outline

- **Overview:** the PISCEES project, the First Order (FO) Stokes model for ice sheets and the *Albany/FELIX* finite element solver.
- **Definitions:** Strong vs. Weak Scalability.
- **Algebraic multi-grid (AMG) preconditioner** based on aggressive semi-coarsening.
- Importance of **node ordering** and **mesh partitioning**.
- **Strong scaling** study for a fine-resolution **Greenland Ice Sheet (GIS)** problem.
- **Weak scaling** study for a moderate-resolution **Antarctic Ice Sheet (AIS)** problem.
- **Summary** and ongoing work.
- **Questions?**

The PISCEES Project and the *Albany/FELIX* Solver

“PISCEES” = Predicting Ice Sheet Climate & Evolution at Extreme Scales
5 Year Project funded by SciDAC, which began in June 2012

Sandia’s Role in the PISCEES Project: to **develop** and **support** a robust and scalable land ice solver based on the “First-Order” (FO) Stokes physics

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***Albany/FELIX* Solver (steady):**
Ice Sheet PDEs (First Order Stokes)
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  - Dynamical core (dycore) when coupled to codes that solve thickness and temperature evolution equations (*CISM/MPAS* codes).

Dycore will provide actionable predictions of 21st century sea-level rise (including uncertainty).

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The First-Order Stokes Model for Ice Sheets & Glaciers

- Ice sheet dynamics are given by the ***"First-Order" Stokes PDEs***: approximation* to viscous incompressible ***quasi-static*** Stokes flow with power-law viscosity.

$$\begin{cases} -\nabla \cdot (2\mu \dot{\boldsymbol{\epsilon}}_1) = -\rho g \dfrac{\partial s}{\partial x} \\ -\nabla \cdot (2\mu \dot{\boldsymbol{\epsilon}}_2) = -\rho g \dfrac{\partial s}{\partial y} \end{cases}, \quad \text{in } \Omega$$

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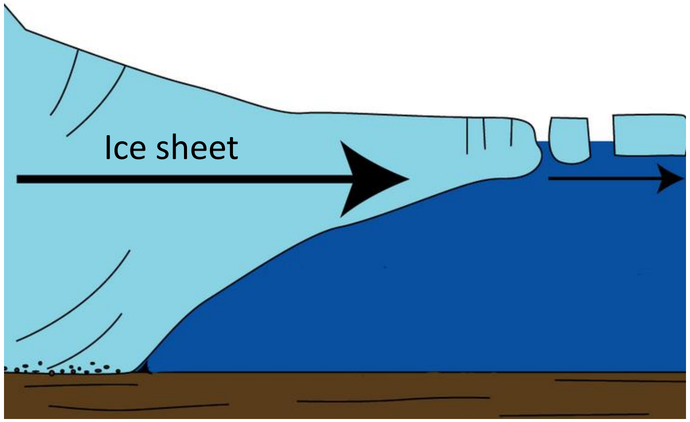
- Viscosity μ is nonlinear function given by "***Glen's law***":

$$\mu = \frac{1}{2} A^{-\frac{1}{n}} \left(\frac{1}{2} \sum_{ij} \dot{\boldsymbol{\epsilon}}_{ij}{}^2 \right)^{\left(\frac{1}{2n} - \frac{1}{2}\right)} \qquad (n = 3)$$

- Relevant boundary conditions:



***Assumption:** aspect ratio δ is small and normals to upper/lower surfaces are almost vertical.

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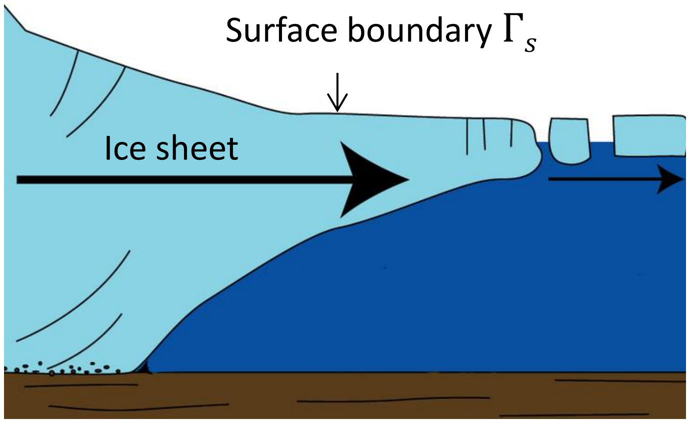

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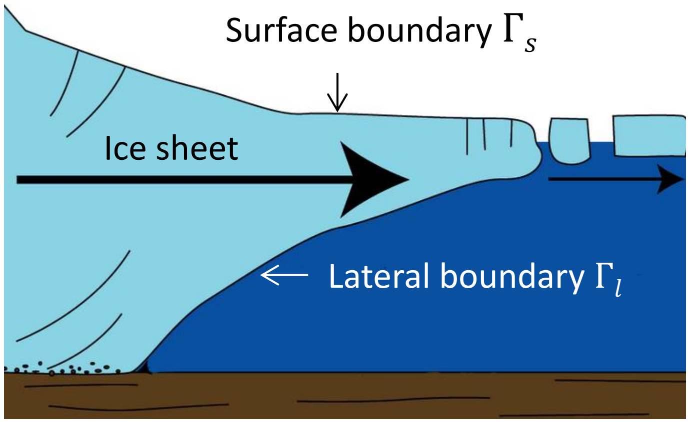
$$2\mu \dot{\boldsymbol{\epsilon}}_i \cdot \boldsymbol{n} = \begin{cases} \rho g z \boldsymbol{n}, & \text{if } z > 0 \\ 0, & \text{if } z \le 0 \end{cases}, \quad \text{on } \Gamma_l$$



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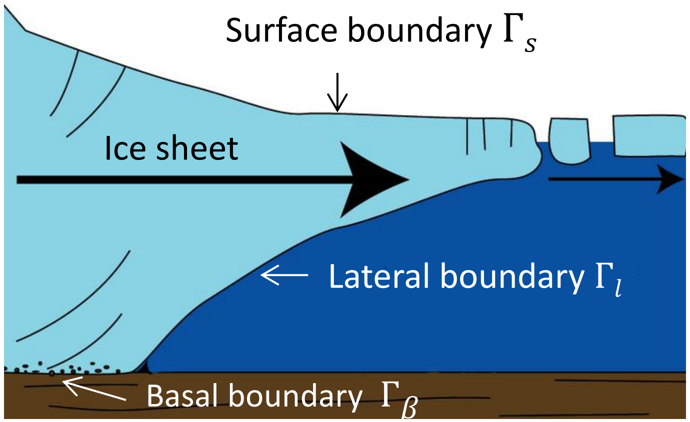
  - ***Basal sliding BC:*** $2\mu\dot{\boldsymbol{\epsilon}}_i \cdot \boldsymbol{n} + \beta u_i = 0$, on Γ_β



$$\beta = \text{sliding coefficient} \ge 0$$

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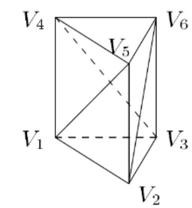
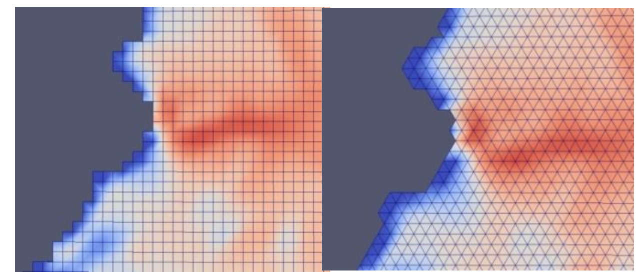
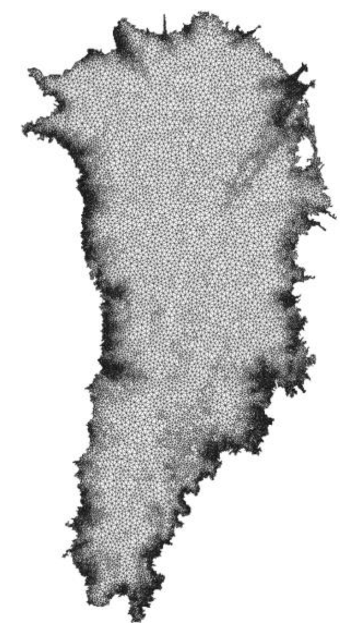
Algorithmic Choices for *Albany/FELIX*: Discretization & Meshes



- **<u>Discretization:</u>** unstructured grid finite element method (FEM)
  - Can handle readily complex geometries.
  - Natural treatment of stress boundary conditions.
  - Enables regional refinement/unstructured meshes.
  - Wealth of software and algorithms.

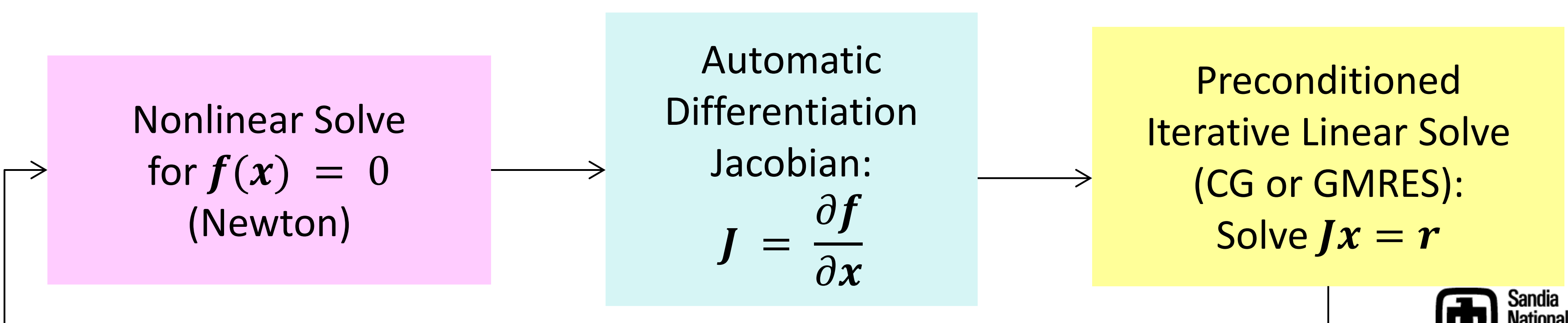


- **<u>Meshes:</u>** can use any mesh but interested specifically in
  - ***Structured hexahedral*** meshes (compatible with *CISM*).
  - ***Structured tetrahedral*** meshes (compatible with *MPAS*)
  - ***Unstructured Delaunay triangle*** meshes with regional refinement based on gradient of surface velocity.
  - All meshes are extruded (structured) in vertical direction as tetrahedra or hexahedra.



Algorithmic Choices for *Albany/FELIX*: Nonlinear & Linear Solver

- **Nonlinear solver:** full Newton with analytic (automatic differentiation) derivatives and homotopy continuation
  - Most robust and efficient for steady-state solves.
  - Jacobian available for preconditioners and matrix-vector products.
  - Analytic sensitivity analysis.
  - Analytic gradients for inversion.
- **Linear solver:** preconditioned iterative method
  - **Solvers:** Conjugate Gradient (CG) or GMRES
  - **Preconditioners:** ILU or algebraic multi-grid (AMG)



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The *Albany/FELIX* Solver: Implementation in *Albany* using *Trilinos*

*Available on `github`: https://github.com/gahansen/Albany (Salinger *et al.*, 2015).

The ***Albany/FELIX*** First Order Stokes solver is implemented in a Sandia (open-source*) parallel C++ finite element code called…

Started by A. Salinger

Land Ice Physics Set (***Albany/FELIX code***)

Other Albany Physics Sets

"Agile Components"

- Discretizations/meshes
- Solver libraries
- Preconditioners
- Automatic differentiation
- Many others!

- Parameter estimation
- Uncertainty quantification
- Optimization
- Bayesian inference

- Configure/build/test/documentation

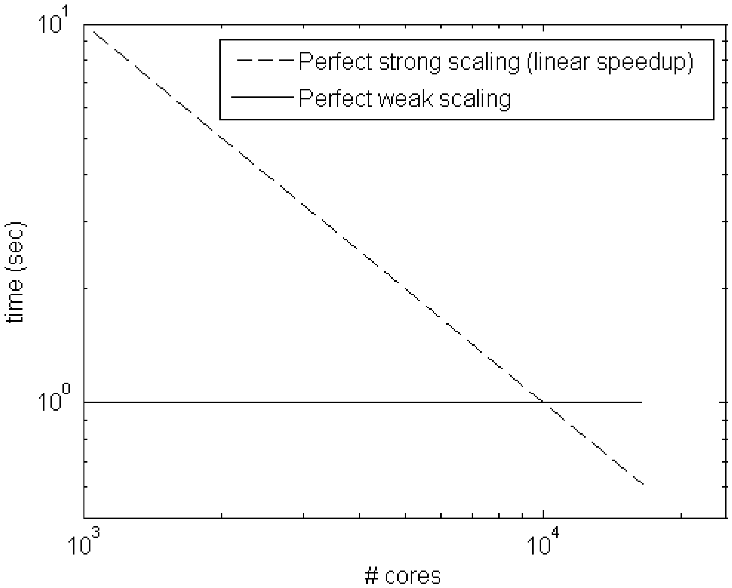
*Use of **Trilinos** components has enabled the **rapid** development of the **Albany/FELIX** First Order Stokes dycore!*

Definitions: Strong vs. Weak Scaling

Scalability (a.k.a. **Scaling Efficiency**) = measure of the efficiency of a code when increasing numbers of parallel processing elements (CPUs, cores, processes, threads, etc.).

- ***Strong scaling:*** how the solution time varies with the number of cores for a fixed total problem size.
  - ⇒ Fix problem size, increase # cores.
  - **Ideal:** linear speed-up with increase in # cores.

- ***Weak scaling:*** how the solution time varies with the number of cores for a fixed problem size per core.
  - ⇒ Increase problem size and # cores s.t. # dofs/core is approximately constant.
  - **Ideal:** solution time remains constant as problem size and # cores increases.



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Scalability via Algebraic Multi-Grid Preconditioning with Semi-Coarsening

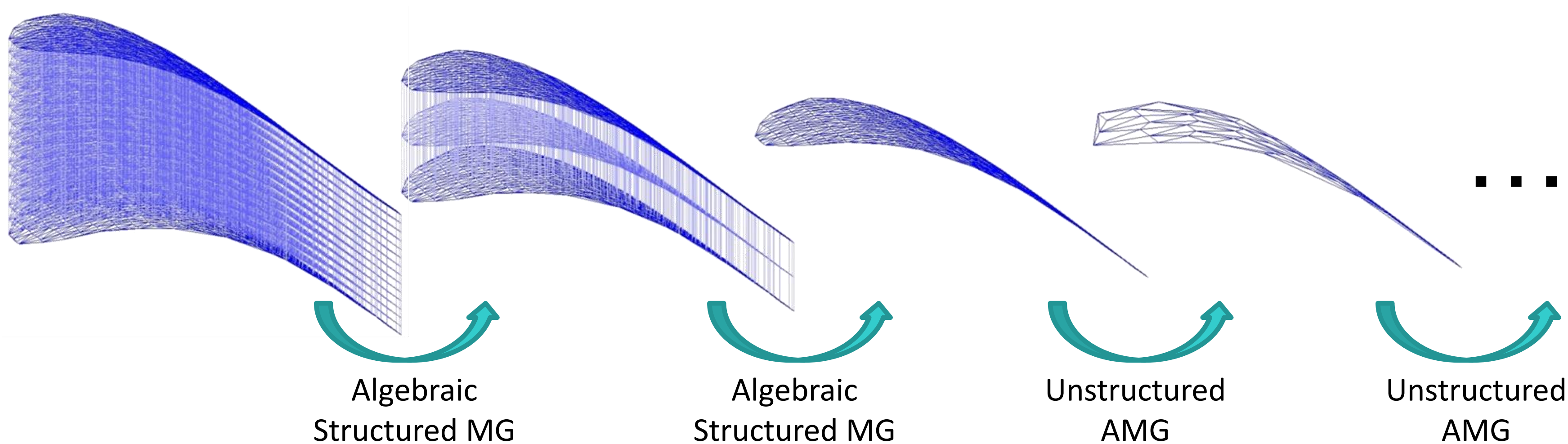
Bad aspect ratios ruin classical AMG convergence rates!

- relatively small horizontal coupling terms, hard to smooth horizontal errors

$\Rightarrow$ Solvers (AMG and ILU) must take aspect ratios into account

We developed a **new AMG solver** based on aggressive **semi-coarsening** *(figure below)*

- Algebraic Structured MG ($\equiv$ matrix depend. MG) used with vertical line relaxation on finest levels + traditional AMG on 1 layer problem



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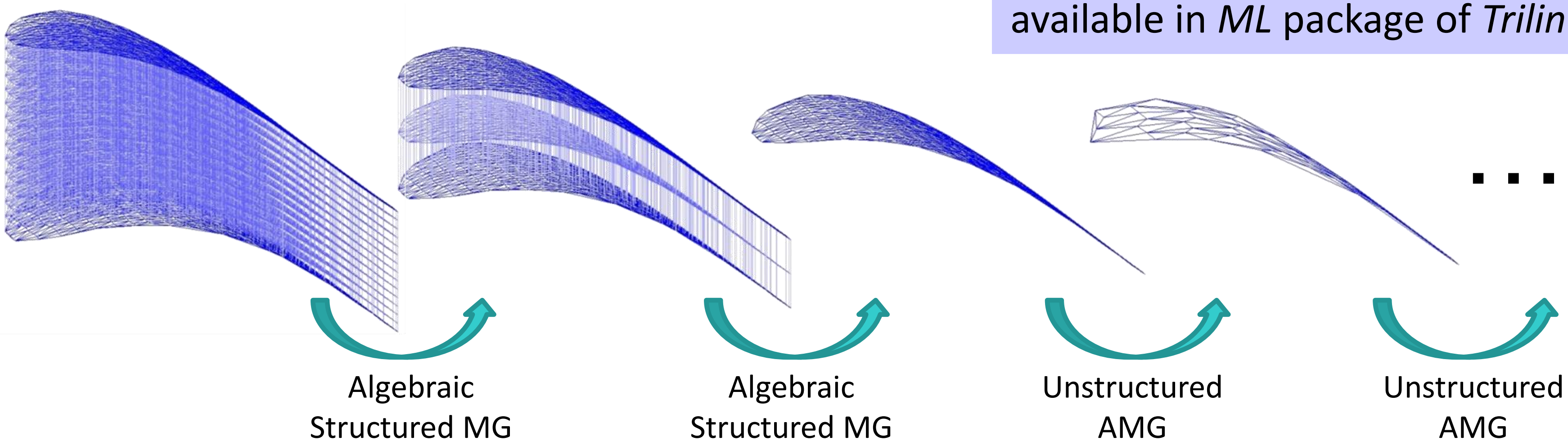

See (Tuminaro, 2014), (Tezaur *et al.*, 2015), (Tuminaro *et al.*, 2015).

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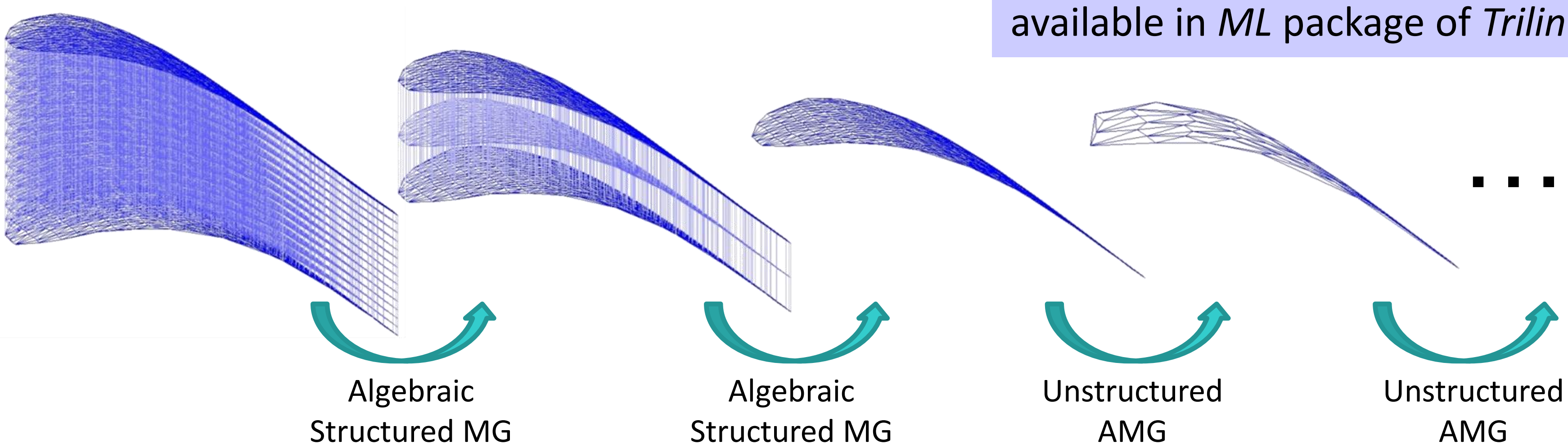

<u>Scaling studies (next slides):</u>
New AMG preconditioner vs. ILU

See (Tuminaro, 2014), (Tezaur *et al.*, 2015), (Tuminaro *et al.*, 2015).

Importance of Node Ordering & Mesh Partitioning

Our studies revealed that **node ordering** and **mesh partitioning** matters for linear solver performance, especially for the ILU preconditioner!

- It is essential that incomplete factorization accurately captures vertical coupling, which is dominant due to anisotropic mesh.

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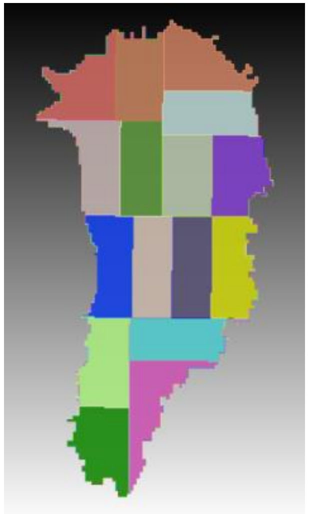

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- This is accomplished by:
  - Ensuring all points along a vertically extruded grid line reside within a single processor ("**2D mesh partitioning**"; top right).

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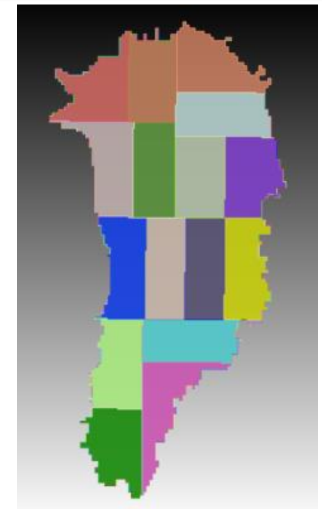

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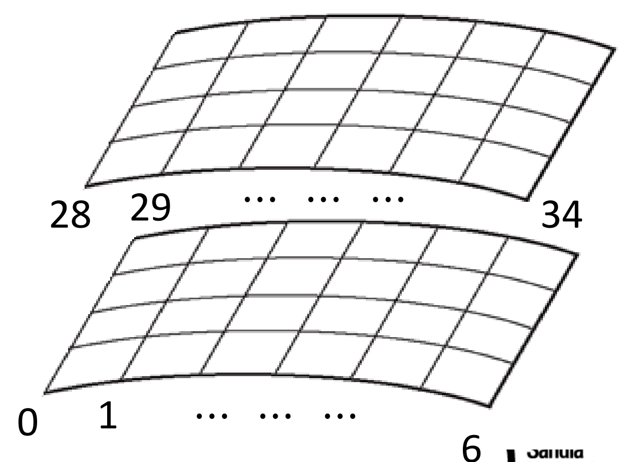
- This is accomplished by:
    - Ensuring all points along a vertically extruded grid line reside within a single processor ("**2D mesh partitioning**"; top right).
    - Ordering the equations such that grid layer k's nodes are ordered before all dofs associated with grid layer $k+1$ ("**row-wise ordering**"; bottom right).



Strong Scaling Study for a Fine-Resolution GIS Problem

- Uniform quadrilateral mesh with 1 km horizontal resolution, extruded vertically using 40 layers (69.8M hex elements, 143M dofs).

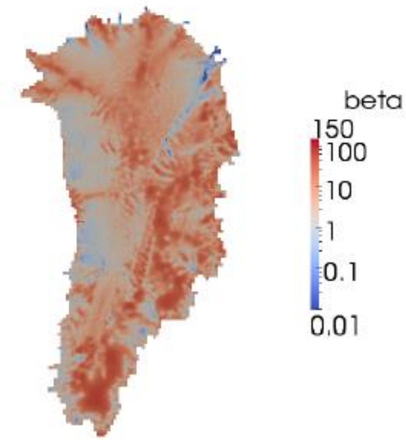
- Run on 1024→16,384 cores of *Hopper* (16-fold increase).

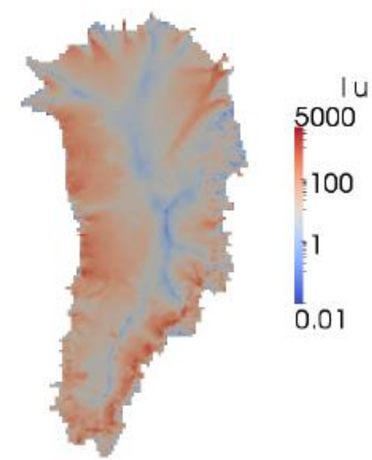
- Realistic basal friction coefficient and bed topographies calculated by solving a deterministic inversion problem that minimized modeled and observed surface velocity mismatch (Perego *et al.*, 2014; top right).

- Realistic 3D temperature field calculated in *CISM* (Shannon *et al.*)

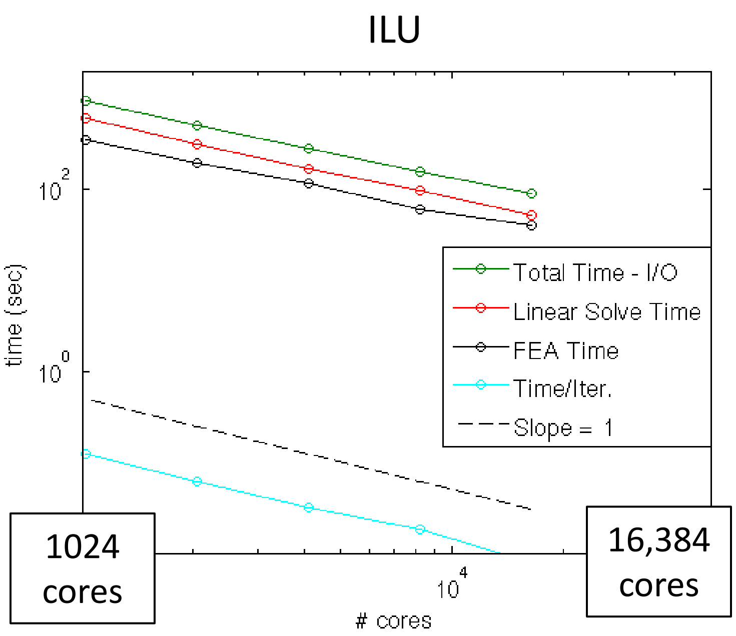
- **Preconditioner:** ILU vs. new AMG (with aggressive semi-coarsening).

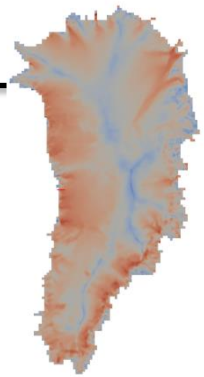
- **Iterative linear solver:** Conjugate Gradient (CG).

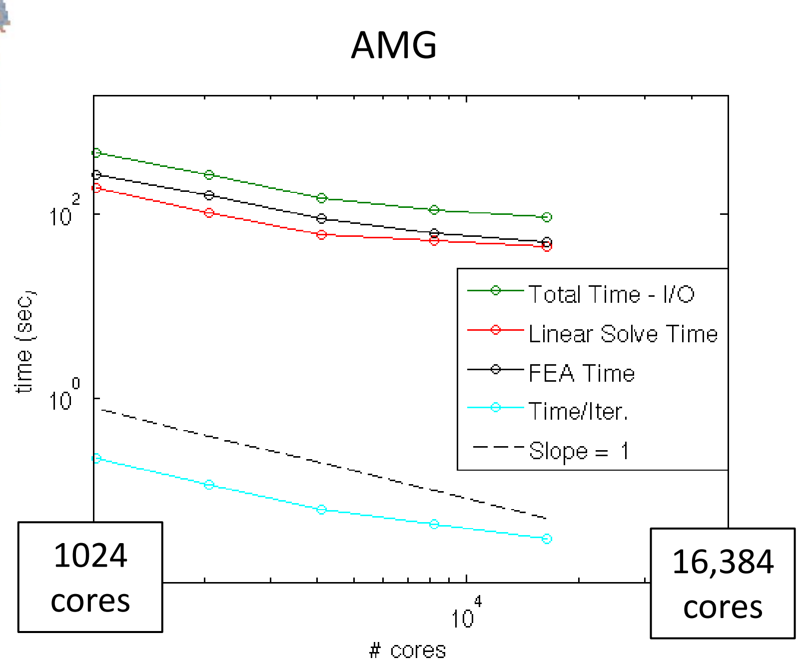




Strong Scaling Study for a Fine-Resolution GIS Problem (cont'd)



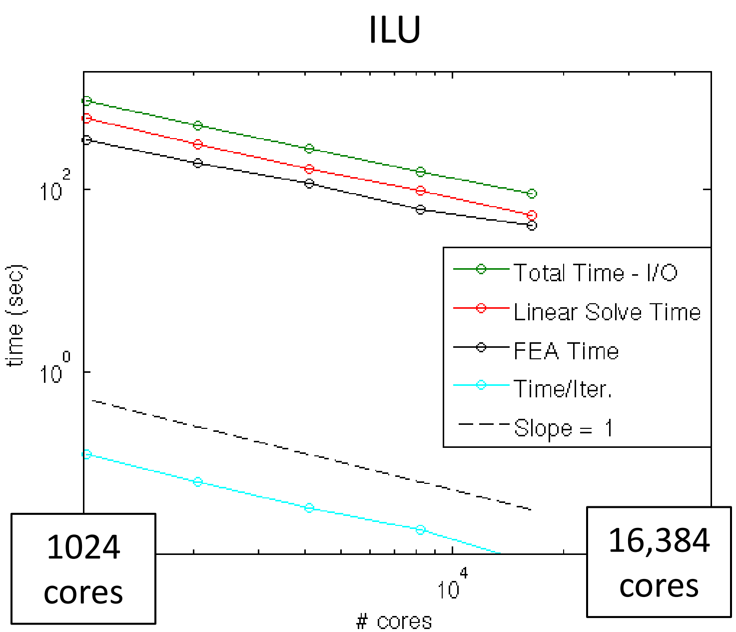


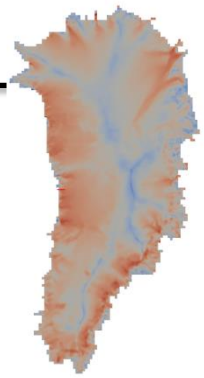


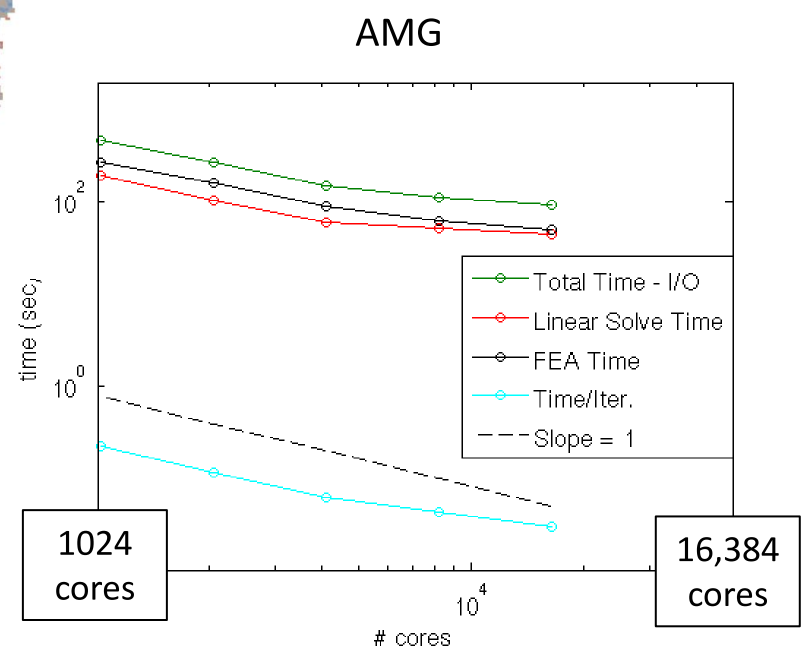
1024 core run:

- AMG preconditioner solves are much faster than ILU (e.g., 194.3 sec for AMG vs. 607.9 sec for ILU).
  - Primarily due to better convergence rate obtained with AMG vs. ILU.

Strong Scaling Study for a Fine-Resolution GIS Problem (cont'd)







<u>16,384 core run:</u>

- ILU preconditioner fairly effective relative to AMG when # dofs/core is modest (e.g., 10K dofs/core).
  - ILU requires slightly more iterations/linear solve but cost/iteration is higher for AMG.
  - AMG solver is very inefficient when # dofs/core is small; communication costs in coarse level processing dominate.

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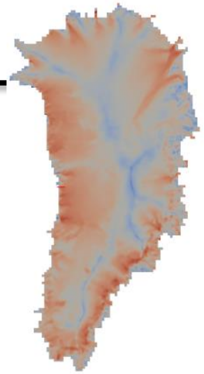
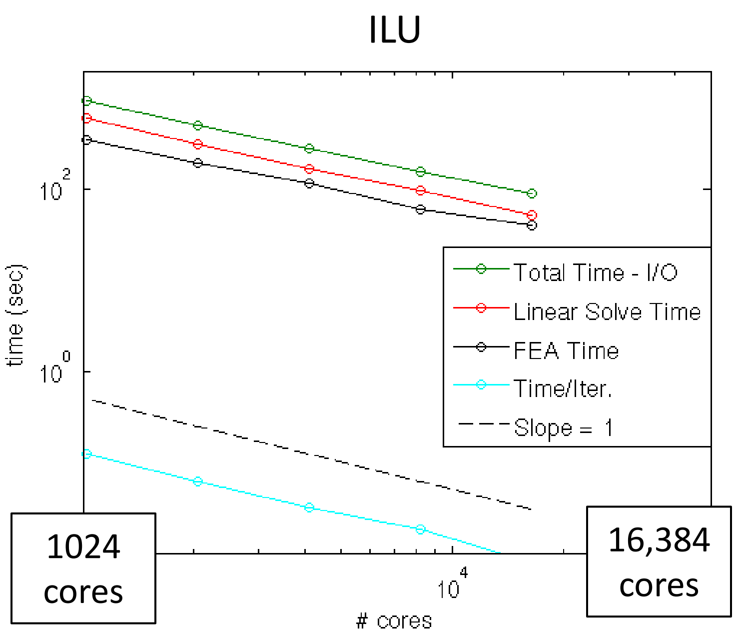
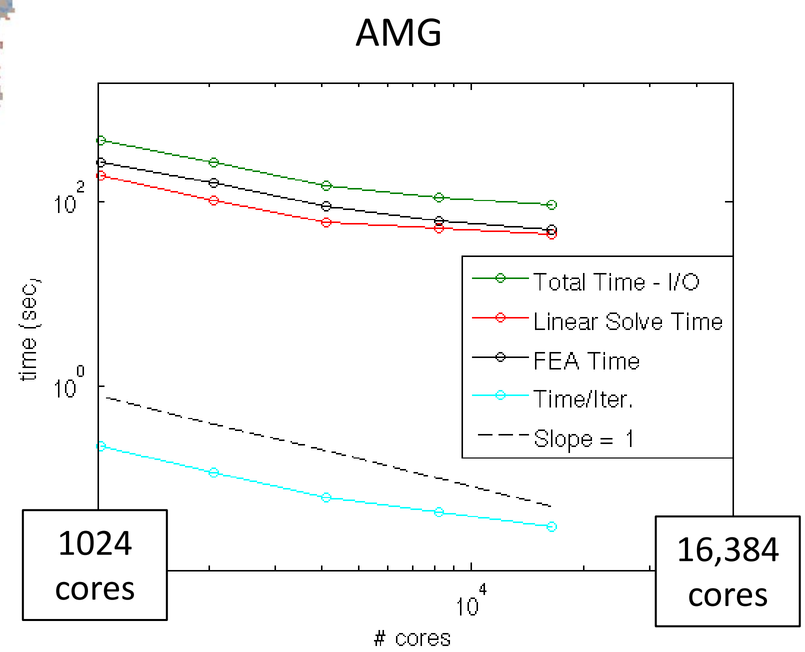
Strong Scaling Study for a Fine-Resolution GIS Problem (cont'd)





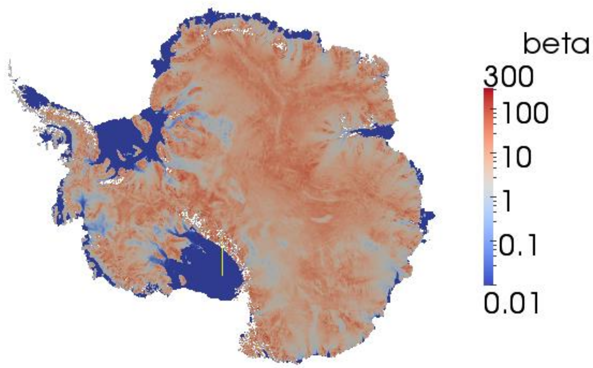


Summary:

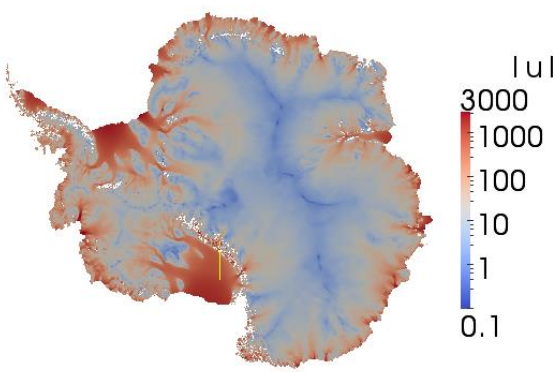
- ILU preconditioner scales better in the strong sense than AMG.
- However, ILU-preconditioned solve is slower for lower #s of cores (more dofs/core).

Weak Scaling Study for a Moderate-Resolution AIS Problem

- 3 hexahedral meshes considered:
  - 8 km horizontal resolution + 5 vertical layers (2.52M dofs) → 16 cores of *Hopper*.
  - 4 km horizontal resolution + 10 vertical layers (18.5M dofs) → 128 cores of *Hopper*.
  - 2 km horizontal resolution + 20 vertical layers (141.5M dofs) → 1024 cores of *Hopper*.



- Ice sheet geometry based on BEDMAP2 (Fretwell *et al*., 2013) and 3D temperature field from (Pattyn, 2010)
- Realistic regularized* basal friction coefficient and bed topographies calculated by solving a deterministic inversion problem that minimizes modeled and observed surface velocity mismatch on finest (2km) resolution geometry (Perego *et al.*, 2014; top right).

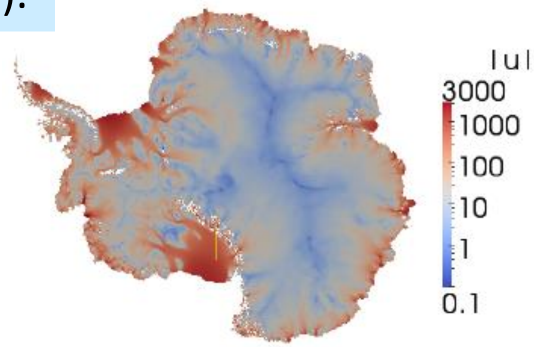


- **Preconditioner:** ILU vs. new AMG (with aggressive semi-coarsening).
- **Iterative linear solver:** GMRES.

*Setting $\beta = \delta > 0$, with $\delta \ll 1$ under ice shelves.

Weak Scaling Study for a Moderate-Resolution AIS Problem (cont'd)

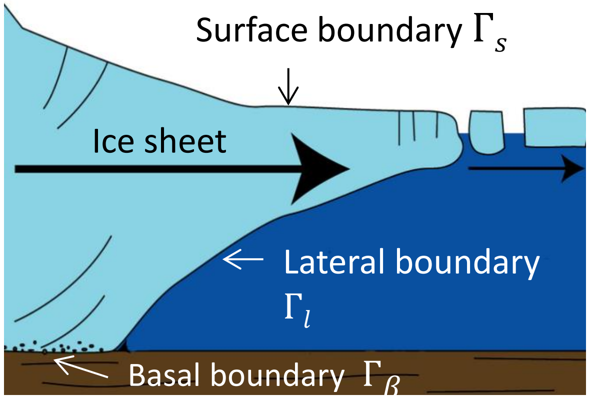
Antarctica is fundamentally different than Greenland:
AIS contains large ice shelves (floating extensions of land ice).



- ***Along ice shelf front:*** open-ocean BC (Neumann).
- ***Along ice shelf base:*** zero traction BC (Neumann).

⇒ For vertical grid lines that lie within ice shelves, top and bottom BCs resemble Neumann BCs so sub-matrix associated with one of these lines is almost* singular.

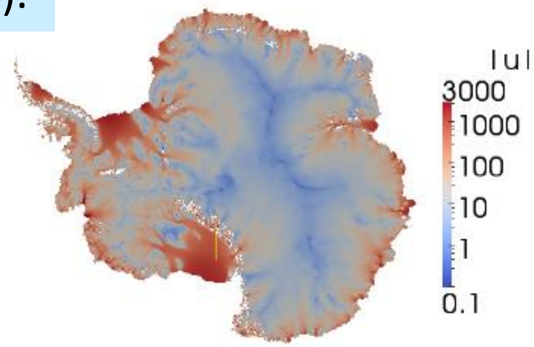
(vertical > horizontal coupling)
+
Neumann BCs
=
nearly singular submatrix associated with vertical lines



*Completely singular in the presence of islands and some ice tongues.

Weak Scaling Study for a Moderate-Resolution AIS Problem (cont'd)

Antarctica is fundamentally different than Greenland:
AIS contains large ice shelves (floating extensions of land ice).



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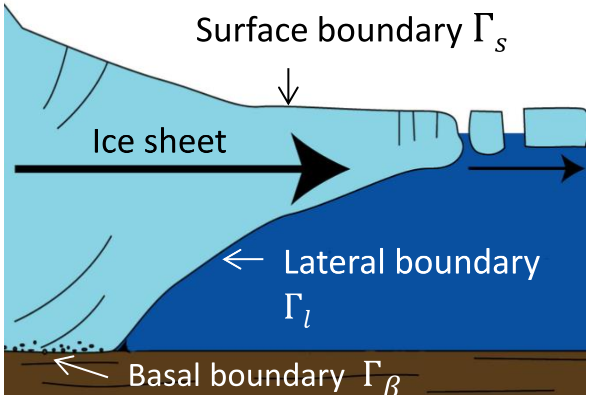
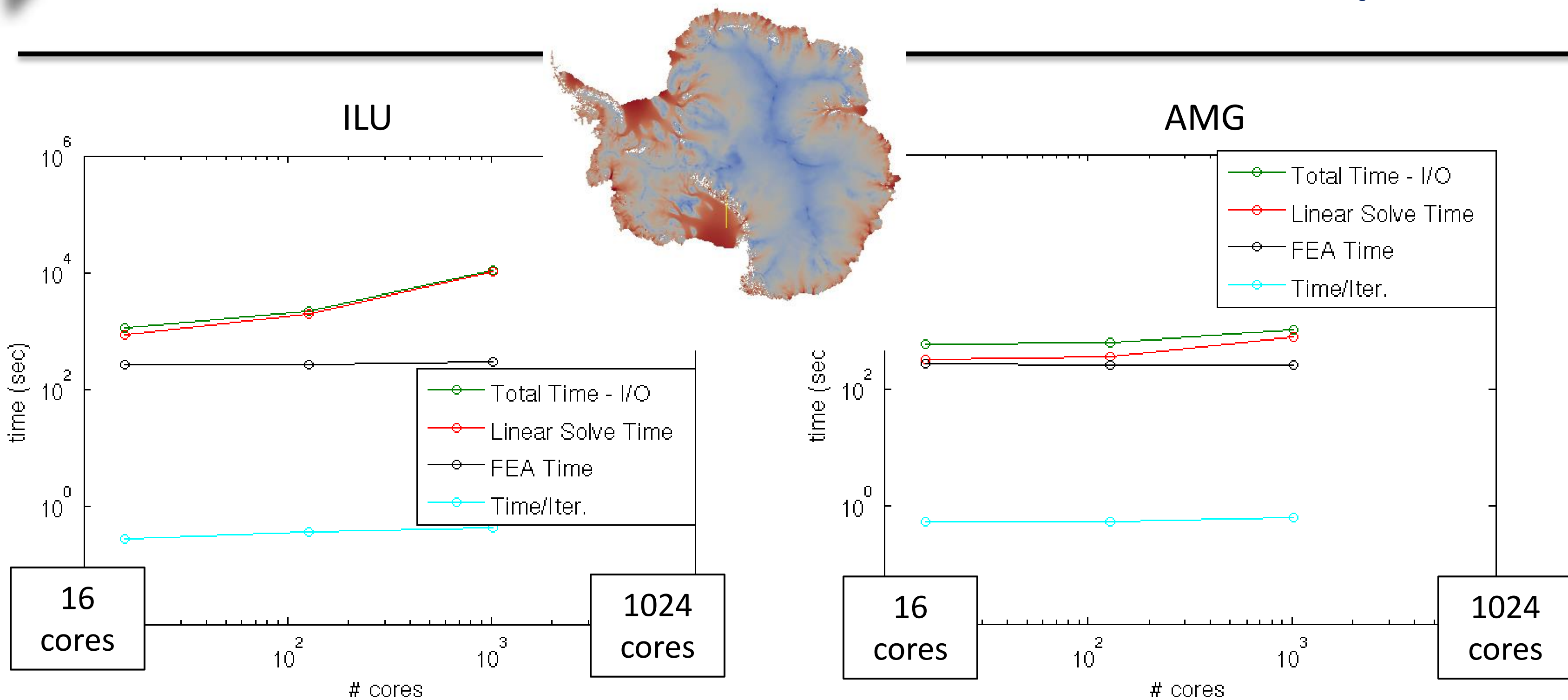


⇒ Ice shelves give rise to severe ill-conditioning of linear systems!

*Completely singular in the presence of islands and some ice tongues.

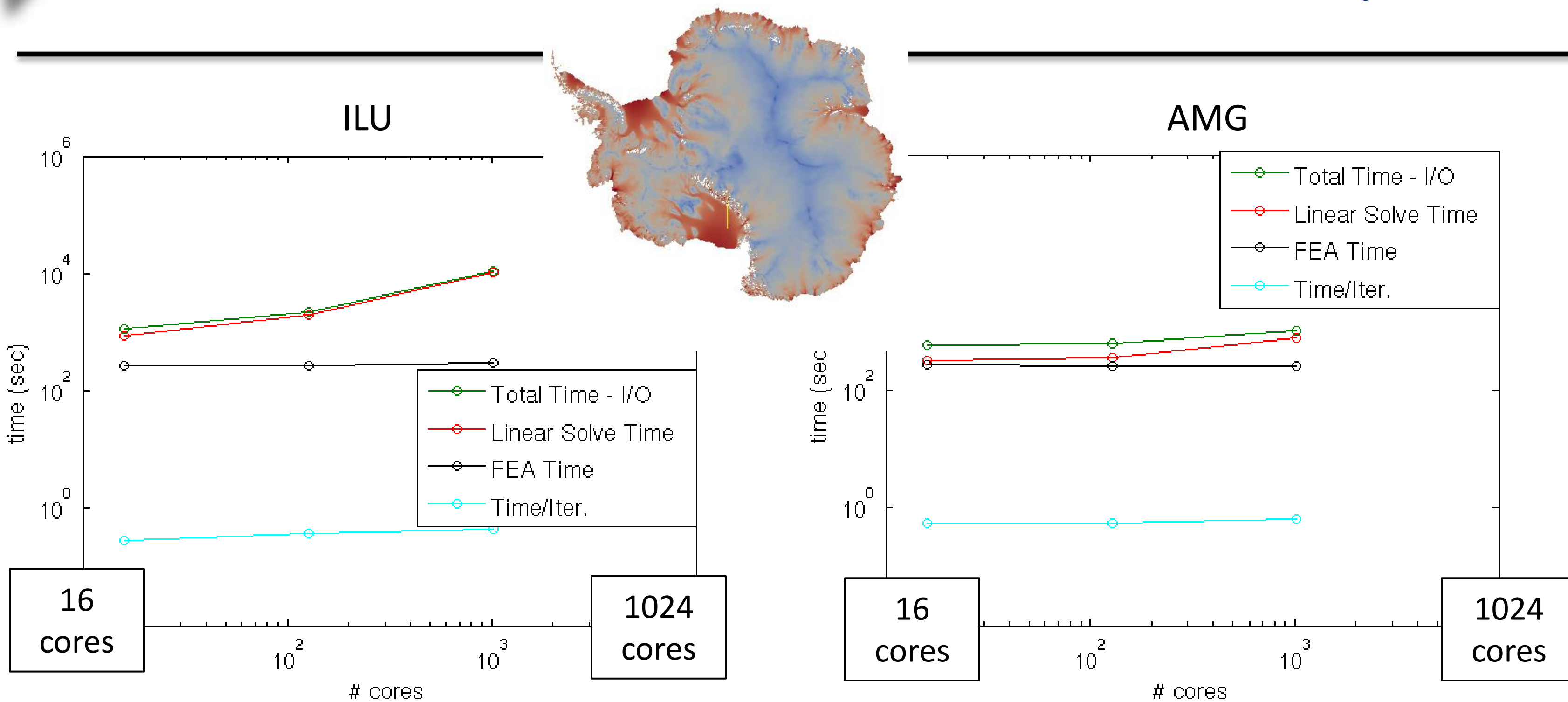
Weak Scaling Study for a Fine-Resolution AIS Problem (cont'd)



ILU vs. AMG:

- ILU solver > 10× slower than AMG solver on 1024 core problem.
  - Due to extremely poor convergence of ILU solver (~700 iterations/solve) → resulting from ill-conditioning of underlying linear systems.
- AMG iterations do grow as problem refined (14.4 iterations/solve on 16 cores vs. 35.5 iterations/solve on 1024 cores), but it is better suited to linear systems associated with AIS.

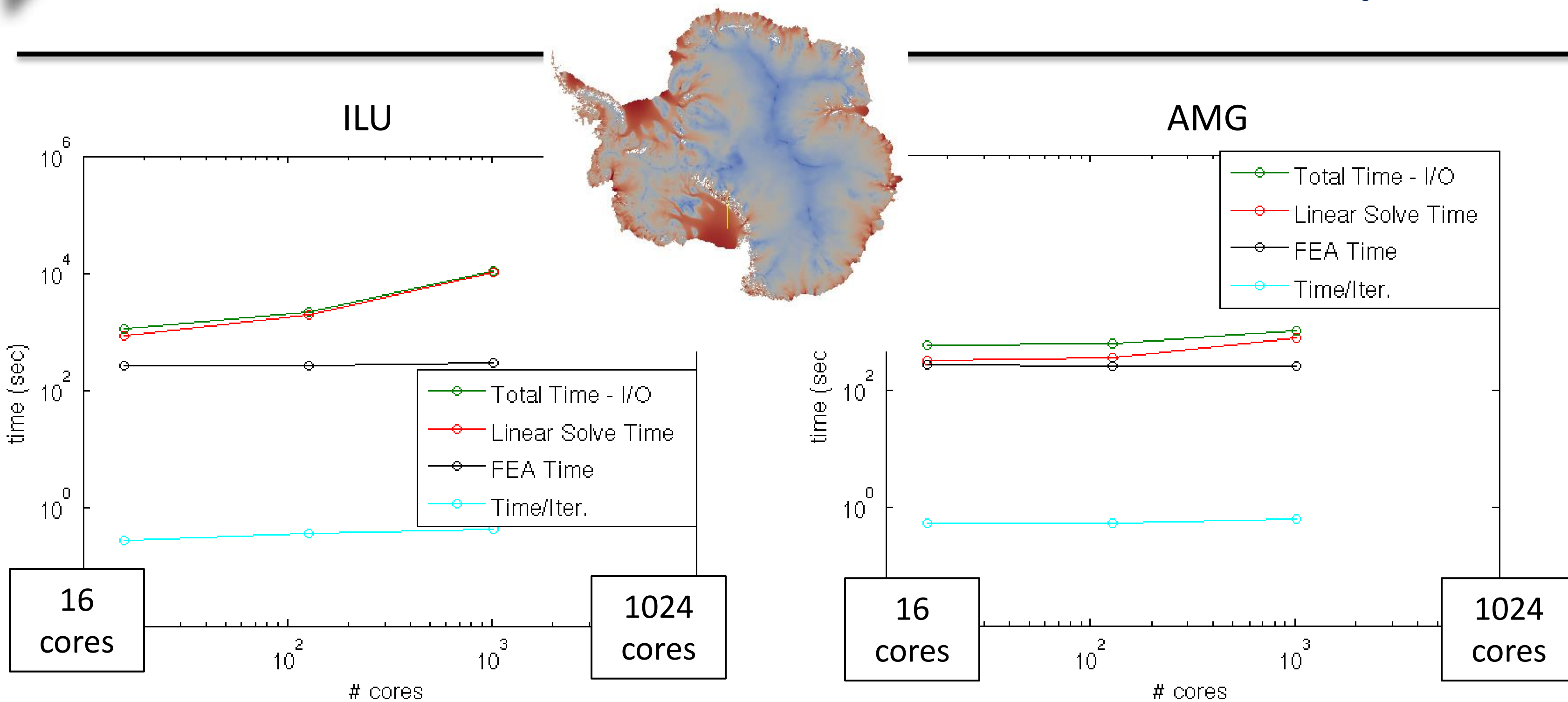
Weak Scaling Study for a Fine-Resolution AIS Problem (cont'd)



GMRES vs. CG:

- GMRES solver found to be more effective than CG, even though problem is symmetric.
  - We believe GMRES is somewhat less sensitive to rounding errors associated with the severe ill-conditioning induced by the presence of ice shelves.
  - GMRES and CG minimize different norms.

Weak Scaling Study for a Fine-Resolution AIS Problem (cont'd)



Summary:

- Severe ill-conditioning caused by ice shelves!
- GMRES less sensitive than CG to rounding errors from ill-conditioning [also minimizes different norm].
- AMG preconditioner less sensitive than ILU to ill-conditioning.

(vertical > horizontal coupling)
+
Neumann BCs
=
nearly singular submatrix associated with vertical lines

Summary and Ongoing Work

Summary:

- This talk described the development of a finite element land ice solver known as *Albany/FELIX* written using the libraries of the *Trilinos* libraries.
- Strong and weak scaling studies on GIS and AIS problems revealed good overall scalability can be achieved by using a new AMG preconditioner based on aggressive semi-coarsening.

I. Tezaur, R. Tuminaro, M. Perego, A. Salinger, S. Price. "On the scalability of the *Albany/FELIX* first-order Stokes approximation ice sheet solver for large-scale simulations of the Greenland and Antarctic ice sheets", *MSESM/ICCS*, Reykjavik, Iceland (June 2015).

Ongoing/future work:

- Dynamic simulations of ice evolution using *CISM-Albany* and *MPAS-Albany*.
- Deterministic and stochastic initialization runs.
- Porting of code to new architecture supercomputers.
- Journal article on AMG preconditioner in preparation for *SISC* (Tuminaro *et. al*, 2015)
- Delivering code to climate community and coupling to earth system models.

Funding/Acknowledgements

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SciDAC Scientific Discovery through Advanced Computing

SUPER INSTITUTE FOR SUSTAINED PERFORMANCE, ENERGY, AND RESILIENCE

PISCEES team members: *W. Lipscomb, S. Price, M. Hoffman, A. Salinger, M. Perego, I. Tezaur, R. Tuminaro, P. Jones, K. Evans, P. Worley, M. Gunzburger, C. Jackson;*

Trilinos/DAKOTA collaborators*: E. Phipps, M. Eldred, J. Jakeman, L. Swiler.*

Thank you! Questions?

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[1] M.A. Heroux *et al.* “An overview of the Trilinos project.” *ACM Trans. Math. Softw.* **31**(3) (2005).

[2] A.G. Salinger *et al*. "Albany: Using Agile Components to Develop a Flexible, Generic Multiphysics Analysis Code", *Comput. Sci. Disc.* (submitted, 2015).

[3] **I. Tezaur**, M. Perego, A. Salinger, R. Tuminaro, S. Price. "*Albany/FELIX*: A Parallel, Scalable and Robust Finite Element Higher-Order Stokes Ice Sheet Solver Built for Advanced Analysis", *Geosci. Model Develop.* 8 (2015) 1-24.

[4] **I. Tezaur**, R. Tuminaro, M. Perego, A. Salinger, S. Price. "On the scalability of the *Albany/FELIX* first-order Stokes approximation ice sheet solver for large-scale simulations of the Greenland and Antarctic ice sheets", *MSESM/ICCS15*, Reykjavik, Iceland (June 2014).

[5] R.S. Tuminaro, **I. Tezaur**, M. Perego, A.G. Salinger. "A Hybrid Operator Dependent Multi-Grid/Algebraic Multi-Grid Approach: Application to Ice Sheet Modeling", *SIAM J. Sci. Comput.* (in prep).

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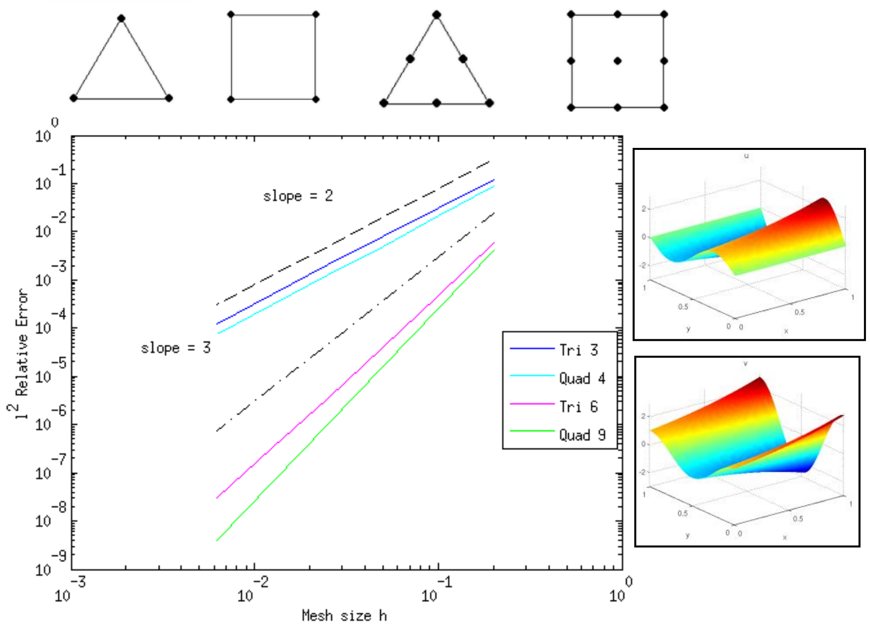
[8] P. Fretwell, *et al.* "BEDMAP2: Improved ice bed, surface, and thickness datasets for Antarctica", *The Cryosphere* 7(1) (2013) 375-393.

[9] F. Pattyn. "Antarctic subglacial conditions inferred from a hybrid ice sheet/ice stream model", *Earth and Planetary Science Letters 295 (2010).*

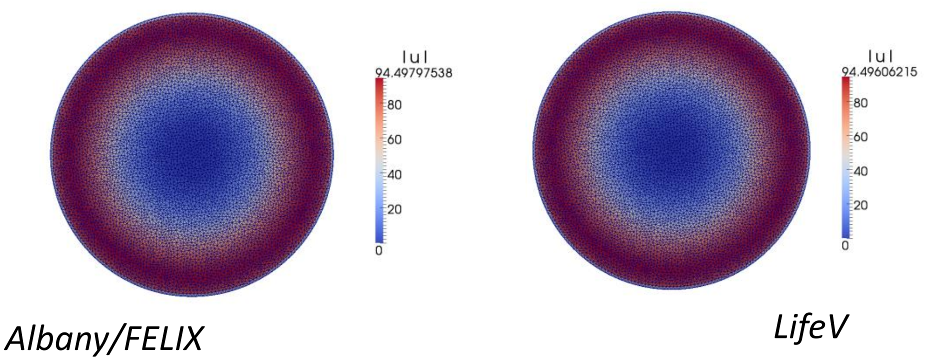
[10] M. Perego, S. Price, G. Stadler. "Optimal Initial Conditions for Coupling Ice Sheet Models to Earth System Models", *J. Geophys. Res.* 119 (2014) 1894-1917.

Appendix: Verification/Mesh Convergence Studies

Stage 1: solution verification on 2D MMS problems we derived.

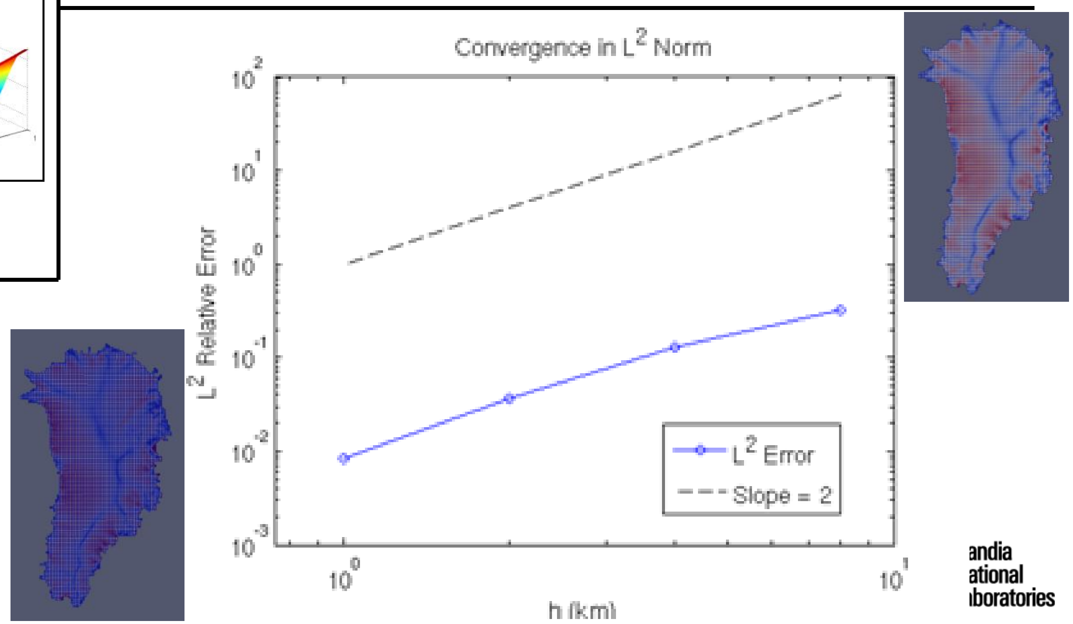


Stage 2: code-to-code comparisons on canonical ice sheet problems.

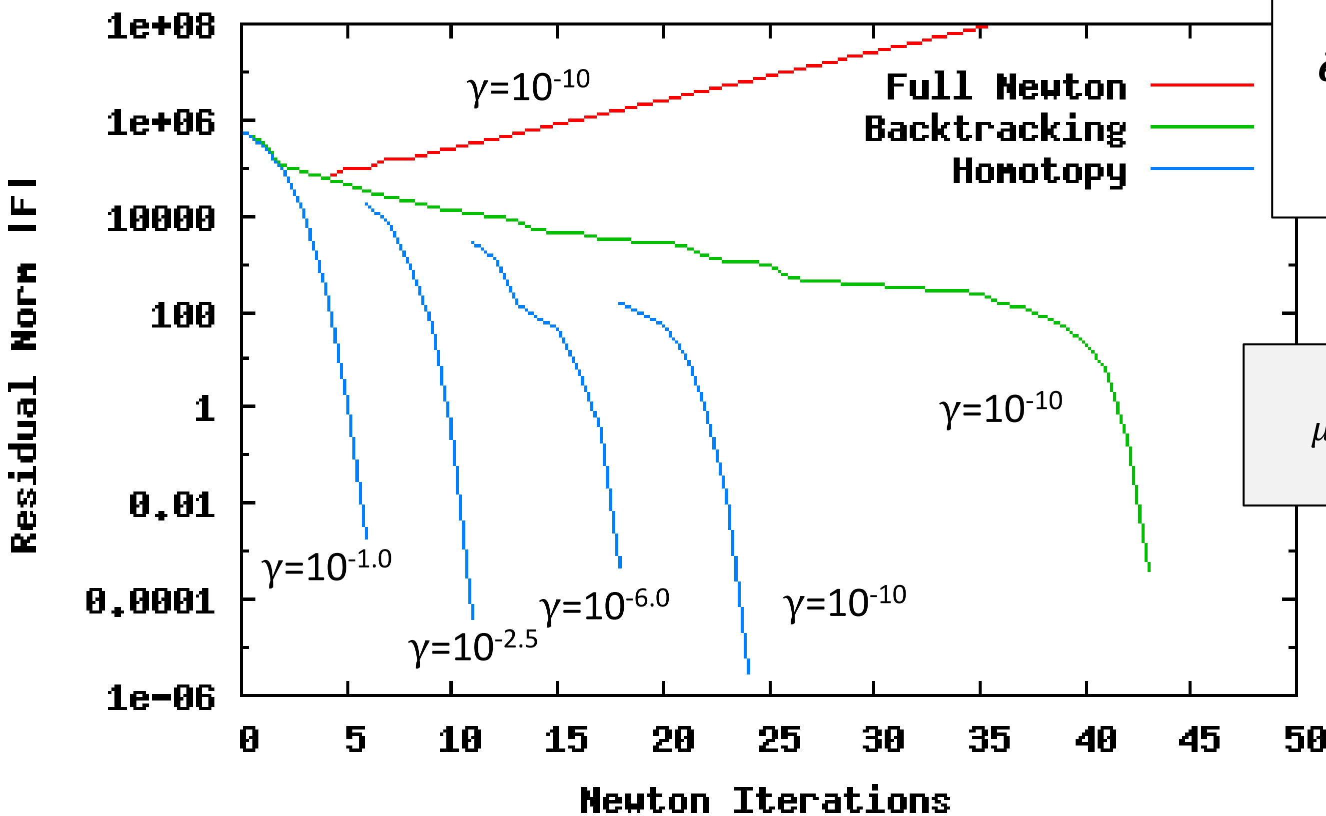


Stage 3: full 3D mesh convergence study on Greenland w.r.t. reference solution.

Are the Greenland problems resolved?
Is theoretical convergence rate achieved?



Appendix: Robustness of Newton's Method via Homotopy Continuation (LOCA)



$$\dot{\epsilon}_1{}^T = (2\dot{\epsilon}_{11} + \dot{\epsilon}_{22}, \dot{\epsilon}_{12}, \dot{\epsilon}_{13})$$
$$\dot{\epsilon}_2{}^T = (2\dot{\epsilon}_{12}, \dot{\epsilon}_{11} + 2\dot{\epsilon}_{22}, \dot{\epsilon}_{23})$$
$$\dot{\epsilon}_{\mathrm{ij}} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial uj}{\partial xi}\right)$$

Glen's Law Viscosity:

$$\mu = \frac{1}{2} A^{-\frac{1}{n}} \left(\frac{1}{2} \sum_{ij} \dot{\epsilon}_{ij}{}^2\right)^{\left(\frac{1}{2n} - \frac{1}{2}\right)}$$

$n = 3$
(Glen's law exponent)

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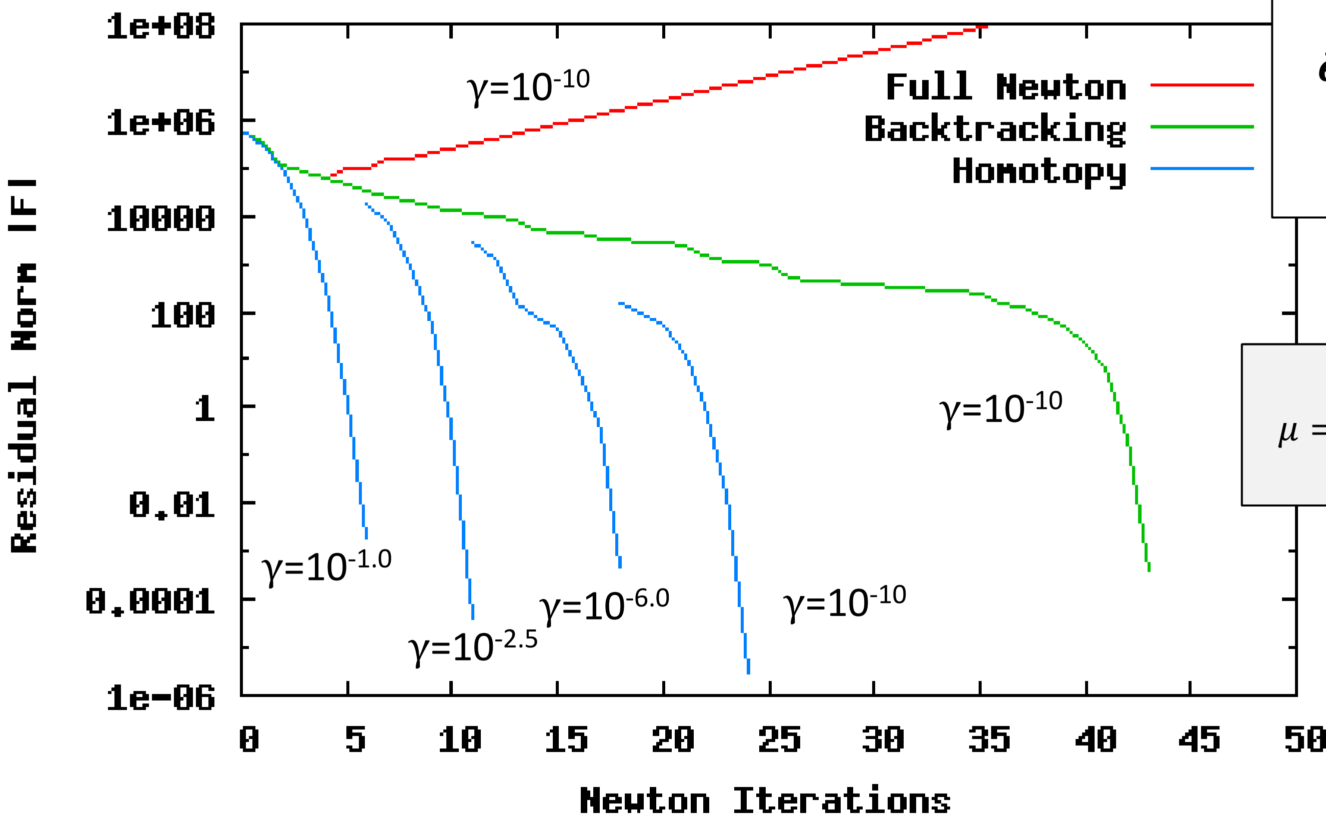

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Glen's Law Viscosity:

$$\mu = \frac{1}{2} A^{-\frac{1}{n}} \left(\frac{1}{2}\sum_{ij} \dot{\epsilon}_{ij}{}^2 + \gamma\right)^{\left(\frac{1}{2n} - \frac{1}{2}\right)}$$

γ = regularization parameter

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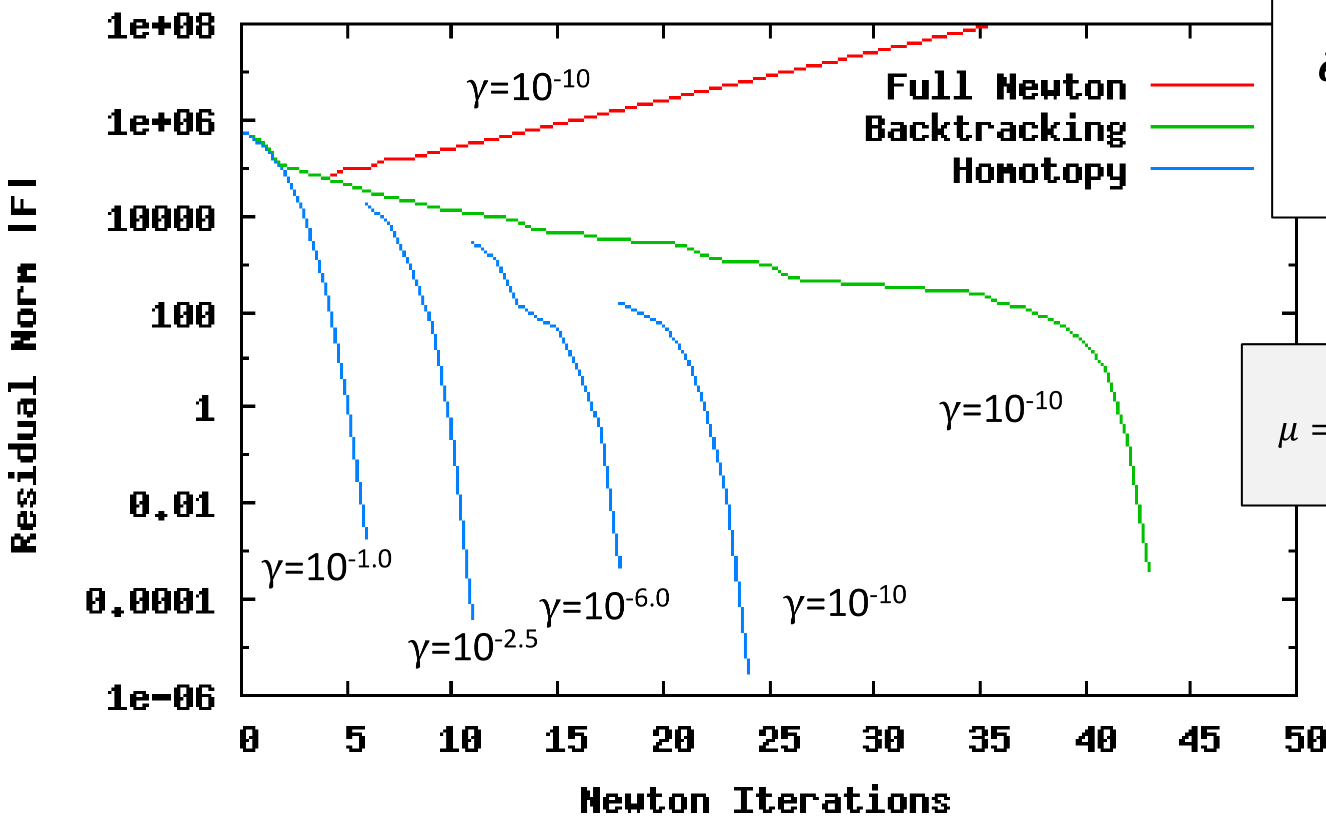

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$\gamma =$ regularization parameter

$n = 3$
(Glen's law exponent)

- Newton's method most robust with full step + homotopy continuation of $\gamma \rightarrow 10^{-10}$: converges out-of-the-box!